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fields
NEWS 15 APR 04 EMBASE - Database reloaded and enhanced

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=> FIL REGISTRY
COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 0.21 0.21

FULL ESTIMATED COST

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 3 TO 163
PROJECTED ANSWERS: 0 TO 0

L8 0 SEA SSS SAM L7

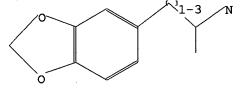
=> s 17 sss full FULL SEARCH INITIATED 12:41:02 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 68 TO ITERATE

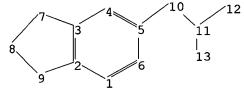
100.0% PROCESSED 68 ITERATIONS 0 ANSWERS

SEARCH TIME: 00.00.01

L9 0 SEA SSS FUL L7

=> Uploading C:\Program Files\Stnexp\Queries\10736018c.str





chain nodes : 10 11 12 13 ring nodes :

1 2 3 4 5 6 7 8 9

chain bonds :

5-10 10-11 11-12 11-13

ring bonds :

1-2 1-6 2-3 2-9 3-4 3-7 4-5 5-6 7-8 8-9

exact/norm bonds :

11-12

exact bonds :

2-9 3-7 5-10 7-8 8-9 10-11 11-13

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems:

containing 1:

G1:H, CH3, Et

G2:CH3,Et,H

Hydrogen count :

1:= exact 1 4:= exact 1 6:= exact 1 8:= exact 2 10:= exact 2 11:= exact 1

13:= exact 3

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS

11:CLASS 12:CLASS 13:CLASS

L10 STRUCTURE UPLOADED

=> s 110

SAMPLE SEARCH INITIATED 12:42:57 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 297 TO ITERATE

10/736,005

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS:

4907 TO 6973

PROJECTED ANSWERS:

145 TO 693

T.11

21 SEA SSS SAM L10

=> s l10 sss full

FULL SEARCH INITIATED 12:43:13 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 5966 TO ITERATE

100.0% PROCESSED 5966 ITERATIONS 598 ANSWERS

SEARCH TIME: 00.00.01

L12

598 SEA SSS FUL L10

=> FIL CAPLUS

COST IN U.S. DOLLARS

SINCE FILE TOTAL

E FILE TOTAL ENTRY SESSION 662.09 662.30

FULL ESTIMATED COST

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FILE COVERS 1907 - 7 Apr 2005 VOL 142 ISS 15 FILE LAST UPDATED: 6 Apr 2005 (20050406/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 112

L13 2101 L12

=> s 113 and determin? or detect?

786021 DETERMIN?

598629 DET

37273 DETS

632931 DET

(DET OR DETS)

1952526 DETD

318256 DETG

1471276 DETN

130107 DETNS

1547459 DETN

(DETN OR DETNS)

3895108 DETERMIN?

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(DETERMIN? OR DET OR DETD OR DETG OR DETN)
       1451462 DETECT?
L14
       1451752 L13 AND DETERMIN? OR DETECT?
=> s 113 and (determin? or detect?)
        786021 DETERMIN?
        598629 DET
         37273 DETS
        632931 DET
                 (DET OR DETS)
       1952526 DETD
        318256 DETG
       1471276 DETN
        130107 DETNS
       1547459 DETN
                 (DETN OR DETNS)
       3895108 DETERMIN?
                 (DETERMIN? OR DET OR DETD OR DETG OR DETN)
       1451462 DETECT?
           731 L13 AND (DETERMIN? OR DETECT?)
L15
=> s 115 and (protein or label)
       1730008 PROTEIN
       1200777 PROTEINS
       2008778 PROTEIN
                 (PROTEIN OR PROTEINS)
         56478 LABEL
         19010 LABELS
         67557 LABEL
                 (LABEL OR LABELS)
L16
            59 L15 AND (PROTEIN OR LABEL)
=> s 116 and (ecstasy or ?amphetamine)
           720 ECSTASY
         23840 ?AMPHETAMINE
L17
            54 L16 AND (ECSTASY OR ?AMPHETAMINE)
=> s 117 and antibody
        275082 ANTIBODY
        318420 ANTIBODIES
        429627 ANTIBODY
                 (ANTIBODY OR ANTIBODIES)
            16 L17 AND ANTIBODY
L18
=> s 118 and immunogen
          5878 IMMUNOGEN
          3272 IMMUNOGENS
          8202 IMMUNOGEN
                 (IMMUNOGEN OR IMMUNOGENS)
             8 L18 AND IMMUNOGEN
L19
=> d l19 ibib abs hitstr tot
L19 ANSWER 1 OF 8 CAPLUS COPYRIGHT 2005 ACS on STN
                        2003:693233 CAPLUS
ACCESSION NUMBER:
DOCUMENT NUMBER:
                         139:207730
TITLE:
                         Antibodies for detecting
                         amphetamine derivatives, compounds useful in
                         antibody production, reagent kits, and
                         detection methods for amphetamine
                         derivatives
                         Hui, Raymond A.
INVENTOR(S):
PATENT ASSIGNEE(S):
                         Roche Diagnostics G.m.b.H., Germany; F. Hoffmann-La
```

Roche A.-G.

SOURCE:

Eur. Pat. Appl., 30 pp.

CODEN: EPXXDW

DOCUMENT TYPE:

Patent English

LANGUAGE:

M COUNTRY 1

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

| PATENT NO. |       |       |       | KIND DATE |            |      |      | APPLICATION NO. |      |      |       |       |      | DATE  |     |       |     |
|------------|-------|-------|-------|-----------|------------|------|------|-----------------|------|------|-------|-------|------|-------|-----|-------|-----|
|            |       |       |       |           |            | -    |      |                 |      |      |       |       |      |       | -   |       |     |
| EP         | 1340  | 981   |       |           | A2         |      | 2003 | 0903            |      | EΡ   | 2003- | -3298 |      |       | 2   | 00302 | 225 |
|            | R:    | AT,   | BE,   | CH,       | DE,        | DK,  | ES,  | FR,             | GB,  | GR   | , IT, | LI,   | LU,  | NL,   | SE, | MC,   | PT, |
|            |       | ΙE,   | SI,   | LT,       | LV,        | FI,  | RO,  | MK,             | CY,  | AL   | , TR, | BG,   | CZ,  | EE,   | HU, | SK    |     |
| US         | 2003  | 17599 | 95    |           | <b>A</b> 1 | (    | 2003 | 0918            | )    | US - | 2002- | 8746  | 9    |       | 2   | 0020  | 301 |
| CA         | 2419  | 696   |       |           | AA         |      | 2003 | 0901            |      | CA   | 2003- | -2419 | 696  |       | 2   | 0030  | 224 |
| JP         | 2004  | 0023  | 16    |           | A2         |      | 2004 | 0108            |      | JΡ   | 2003- | -4992 | 4    |       | 2   | 0030  | 226 |
| PRIORITY   | APP   | LN.   | INFO  | . :       |            |      |      |                 |      | US   | 2002- | -8746 | 9    | i     | A 2 | 0020  | 301 |
| OTHER SO   | URCE  | (S):  |       |           | MARI       | PAT  | 139: | 2077            | 30   |      |       |       |      |       |     |       |     |
| AB Con     | npds. | inc   | Ludi  | ng ha     | apter      | ıs,  | inte | rmed:           | iate | s,   | and i | mmun  | ogen | s tha | at  |       |     |
| are        | use   | ful : | in tl | he p      | roduc      | ctic | n of | ant:            | ibod | ies  | spec  | cific | for  | the   |     |       |     |
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are useful in the production of antibodies specific for the methylenedioxy class of amphetamine derivs. are described.

Antibodies specific for the methylenedioxy class of amphetamine derivs., reagent kits containing antibodies specific for the methylenedioxy class of amphetamine derivs., methods of producing antibodies specific for the methylenedioxy class of amphetamine derivs., and methods of detecting analytes including members of the methylenedioxy class of amphetamine derivs. are also described.

IT 4764-17-4, MDA 42542-10-9, MDMA 42542-10-9D, Ecstasy, derivs. 74698-36-5, MDPA 82801-81-8, MDEA

RL: ANT (Analyte); ANST (Analytical study)
(antibodies for detecting amphetamine
derivs., compds. for antibody production, reagent kits, and
detection methods for amphetamine derivs.)

RN 4764-17-4 CAPLUS

CN 1,3-Benzodioxole-5-ethanamine, α-methyl- (9CI) (CA INDEX NAME)

RN 42542-10-9 CAPLUS

CN 1,3-Benzodioxole-5-ethanamine,  $N,\alpha$ -dimethyl- (9CI) (CA INDEX NAME)

RN 42542-10-9 CAPLUS

CN 1,3-Benzodioxole-5-ethanamine,  $N,\alpha$ -dimethyl- (9CI) (CA INDEX NAME)

RN 74698-36-5 CAPLUS

CN 1,3-Benzodioxole-5-ethanamine,  $\alpha$ -methyl-N-propyl- (9CI) (CA INDEX NAME)

RN 82801-81-8 CAPLUS

CN 1,3-Benzodioxole-5-ethanamine, N-ethyl- $\alpha$ -methyl- (9CI) (CA INDEX NAME)

IT 590346-15-9DP, carrier protein conjugates

RL: BUU (Biological use, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)

(antibodies for detecting amphetamine

derivs., compds. for antibody production, reagent kits, and

detection methods for amphetamine derivs.)

RN 590346-15-9 CAPLUS

CN Acetamide, N-[2-(1,3-benzodioxol-5-yl)-1-methylethyl]-N-[4-[(2,5-dioxo-1-pyrrolidinyl)oxy]-4-oxobutyl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)

IT 590346-12-6

RL: RCT (Reactant); RACT (Reactant or reagent)

(antibodies for detecting amphetamine

derivs., compds. for antibody production, reagent kits, and

detection methods for amphetamine derivs.)

RN 590346-12-6 CAPLUS

CN 1,3-Benzodioxole-5-ethanamine,  $\alpha$ -methyl-, hydrobromide (9CI) (CA INDEX NAME)

HBr

# IT 590346-11-5P 590346-13-7P 590346-14-8P

590346-15-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(antibodies for detecting amphetamine

derivs., compds. for antibody production, reagent kits, and

detection methods for amphetamine derivs.)

RN 590346-11-5 CAPLUS

CN Butanoic acid, 4-[[2-(1,3-benzodioxol-5-yl)-1-methylethyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

RN 590346-13-7 CAPLUS

CN Butanoic acid, 4-[[2-(1,3-benzodioxol-5-yl)-1-methylethyl](trifluoroacetyl)amino]-, ethyl ester (9CI) (CA INDEX NAME)

RN 590346-14-8 CAPLUS

CN Butanoic acid, 4-[[2-(1,3-benzodioxol-5-yl)-1-methylethyl](trifluoroacetyl)amino]- (9CI) (CA INDEX NAME)

RN 590346-15-9 CAPLUS

CN Acetamide, N-[2-(1,3-benzodioxol-5-yl)-1-methylethyl]-N-[4-((2,5-dioxo-1-pyrrolidinyl)oxy]-4-oxobutyl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)

IT 66142-89-0

RL: ANT (Analyte); BSU (Biological study, unclassified); ANST (Analytical study); BIOL (Biological study)

(cross-reactivity; antibodies for detecting

amphetamine derivs., compds. for antibody production, reagent kits, and detection methods for amphetamine

derivs.)

RN 66142-89-0 CAPLUS

CN 1,3-Benzodioxole-5-ethanamine, N, $\alpha$ -dimethyl-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

L19 ANSWER 2 OF 8 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2003:693232 CAPLUS

DOCUMENT NUMBER: 139:207729

TITLE: Amphetamine derivatives, antibodies

to the derivatives, reagent kits, methods of producing

the antibodies, and methods of

detecting the derivatives

INVENTOR(S):
PATENT ASSIGNEE(S):

Hui, Raymond A.; Root, Richard T.; Vitone, Stephan S. Roche Diagnostics G.m.b.H., Germany; F. Hoffmann-La

Roche A.-G.

SOURCE: Eur. Pat. Appl., 34 pp.

CODEN: EPXXDW

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

DATE APPLICATION NO. DATE PATENT NO. KIND -----\_\_\_\_ \_\_\_\_\_ -----EP 1340980 A1 **₹ 20030903** . EP 2003-3297 20030225 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK US 2003170917 A1 20030911 US 2002-87612 20020301 20030901 CA 2003-2419698 20030224 CA 2419698 AA JP 2004123692 20040422 JP 2003-49992 20030226 A2 US 2002-87612 A 20020301 PRIORITY APPLN. INFO.: MARPAT 139:207729 OTHER SOURCE(S):

AB Compds. including haptens, intermediates, and immunogens that are useful in the production of antibodies specific for the methylenedioxy class of amphetamine derivs. are described.

Antibodies specific for the methylenedioxy class of amphetamine derivs., reagent kits containing antibodies specific for the methylenedioxy class of amphetamine derivs., methods of producing antibodies specific for the methylenedioxy class of amphetamine derivs., and methods of detecting analytes including members of the methylenedioxy class of amphetamine derivs. are also described.

IT 42542-10-9, Ecstasy 42542-10-9D,
Ecstasy, derivs. 82801-81-8, MDEA
RL: ANT (Analyte); ANST (Analytical study)
(amphetamine derivs., anti-derivative antibodies,
reagent kits, antibody production, and derivative detection
methods)

RN 42542-10-9 CAPLUS CN 1,3-Benzodioxole-5-ethanamine, N,α-dimethyl- (9CI) (CA INDEX NAME)

RN 42542-10-9 CAPLUS CN  $1,3-Benzodioxole-5-ethanamine, N,<math>\alpha$ -dimethyl- (9CI) (CA INDEX NAME)

RN 82801-81-8 CAPLUS CN 1,3-Benzodioxole-5-ethanamine, N-ethyl- $\alpha$ -methyl- (9CI) (CA INDEX NAME)

590346-15-9DP, carrier protein conjugates IT

RL: BUU (Biological use, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)

(amphetamine derivs., anti-derivative antibodies,

reagent kits, antibody production, and derivative detection

methods)

590346-15-9 CAPLUS RN

Acetamide, N-[2-(1,3-benzodioxol-5-yl)-1-methylethyl]-N-[4-[(2,5-dioxo-1-1)-1-methylethyl]]CN pyrrolidinyl)oxy]-4-oxobutyl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)

IT 590346-12-6

> RL: RCT (Reactant); RACT (Reactant or reagent) (amphetamine derivs., anti-derivative antibodies,

reagent kits, antibody production, and derivative detection

methods) 590346-12-6 CAPLUS RN

1,3-Benzodioxole-5-ethanamine,  $\alpha$ -methyl-, hydrobromide (9CI) (CA CN INDEX NAME)

$$\begin{array}{c} ^{\rm NH_2} \\ | \\ ^{\rm Me-CH-CH_2} \end{array}$$

### ● HBr

IT 590346-11-5P 590346-13-7P 590346-14-8P

590346-15-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(amphetamine derivs., anti-derivative antibodies,

reagent kits, antibody production, and derivative detection methods)

RN 590346-11-5 CAPLUS

Butanoic acid, 4-[[2-(1,3-benzodioxol-5-yl)-1-methylethyl]amino]-, ethyl CN ester (9CI) (CA INDEX NAME)

RN 590346-13-7 CAPLUS

CN Butanoic acid, 4-[[2-(1,3-benzodioxol-5-yl)-1-methylethyl](trifluoroacetyl)amino]-, ethyl ester (9CI) (CA INDEX NAME)

RN 590346-14-8 CAPLUS

CN Butanoic acid, 4-[[2-(1,3-benzodioxol-5-yl)-1-methylethyl](trifluoroacetyl)amino]- (9CI) (CA INDEX NAME)

RN 590346-15-9 CAPLUS

CN Acetamide, N-[2-(1,3-benzodioxol-5-yl)-1-methylethyl]-N-[4-[(2,5-dioxo-1-pyrrolidinyl)oxy]-4-oxobutyl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)

# IT 66142-89-0 74698-36-5, MDPA

RL: ANT (Analyte); BSU (Biological study, unclassified); ANST (Analytical study); BIOL (Biological study)

(cross-reactivity; amphetamine derivs., anti-derivative antibodies, reagent kits, antibody production, and derivative detection methods)

66142-89-0 CAPLUS RN

1,3-Benzodioxole-5-ethanamine,  $N,\alpha$ -dimethyl-,  $(\alpha S)$ - (9CI) (CA CN INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN74698-36-5 CAPLUS

1,3-Benzodioxole-5-ethanamine, α-methyl-N-propyl- (9CI) CN (CA INDEX NAME)

IT 4764-17-4P, MDA

> RL: ANT (Analyte); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); ANST (Analytical study); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent) (cross-reactivity; amphetamine derivs., anti-derivative

antibodies, reagent kits, antibody production, and derivative detection methods)

RN 4764-17-4 CAPLUS

1,3-Benzodioxole-5-ethanamine, \alpha-methyl- (9CI) (CA INDEX NAME) CN

$$\begin{array}{c} \text{NH}_2 \\ | \\ \text{Me-CH-CH}_2 \\ \end{array}$$

REFERENCE COUNT: THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 3 OF 8 CAPLUS COPYRIGHT 2005 ACS on STN

2003:488680 CAPLUS ACCESSION NUMBER:

139:48560 DOCUMENT NUMBER:

Method and kit for detecting, or TITLE:

determining, 3,4-

methylenedioxymethamphetamine

INVENTOR(S): Mcconnell, Robert Ivan; Benchikh, El Ouard; Fitzgerald, Stephen P.; Lamont, John Victor

PATENT ASSIGNEE(S): Randox Laboratories Ltd., UK

SOURCE: Eur. Pat. Appl., 25 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

| PATENT NO.             | KIND       | DATE      | APPLICATION NO.         | DATE        |  |  |
|------------------------|------------|-----------|-------------------------|-------------|--|--|
|                        |            |           |                         |             |  |  |
| EP 1321772             | <b>A</b> 1 | 20030625  | EP 2002-80462           | 20021217    |  |  |
| R: AT, BE, CH,         | DE, DK     | , ES, FR, | GB, GR, IT, LI, LU, NL, | SE, MC, PT, |  |  |
| IE, SI, LT,            | LV, FI     | , RO, MK, | CY, AL, TR, BG, CZ, EE, | SK          |  |  |
| CN 1429844             | Α          | 20030716  | CN 2002-139960          | 20021220    |  |  |
| US 2004121400          | A1         | 20040624  | US 2002-326742          | 20021220    |  |  |
| PRIORITY APPLN. INFO.: |            |           | EP 2001-205058          | A 20011220  |  |  |
| OTHER SOURCE(S):       | MARPAT     | 139:48560 | )                       |             |  |  |

The present invention describes a hapten derivatized with a crosslinker at the N-position of 3,4-methylenedioxymethamphetamine (MDMA). present invention provides an immunogen comprising the aforementioned hapten, coupled to an antigenicity-conferring carrier material, as well as, conjugates comprising the aforementioned hapten covalently bonded to a detectable labeling agent. In addition, the present invention concerns antibodies raised against the aforementioned immunogens. Finally, the present invention relates to methods and kits for detecting or determining MDMA and N-alkylated derivs. of methylenedioxyamphetamine in biol. fluids. The antibodies of the present invention do not significantly cross-react with amphetamine and methamphetamine. Haptens and immunogens and horseradish peroxidase-labeled hapten reagents were prepared from (3,4methylenedioxy) phenylacetic acid for the development of competitive ELISAs for MDMA.

IT 4764-17-4, MDA 82801-81-8, 3,4-

 ${\tt Methylenedioxyethylamphetamine}$ 

RL: BSU (Biological study, unclassified); BIOL (Biological study) (antibody cross-reactivity with; immunoassay, haptens, reagents and kit for determining 3,4-

methylenedioxymethamphetamine in body fluids)

RN 4764-17-4 CAPLUS

CN 1,3-Benzodioxole-5-ethanamine,  $\alpha$ -methyl- (9CI) (CA INDEX NAME)

RN 82801-81-8 CAPLUS

CN 1,3-Benzodioxole-5-ethanamine, N-ethyl- $\alpha$ -methyl- (9CI) (CA INDEX NAME)

IT 547713-13-3P 547713-15-5P 547713-16-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(as hapten; immunoassay, haptens, reagents and kit for determining

# 3,4-methylenedioxymethamphetamine in body fluids)

RN 547713-13-3 CAPLUS

CN Butanoic acid, 4-[[2-(1,3-benzodioxol-5-yl)-1-methylethyl]methylamino]-(9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \mid \\ \text{HO}_2\text{C} - \left(\text{CH}_2\right)_3 - \text{N} \\ \mid \\ \text{Me} - \text{CH} - \text{CH}_2 \\ \end{array}$$

RN 547713-15-5 CAPLUS

CN 1,4-Butanediamine, N-[2-(1,3-benzodioxol-5-yl)-1-methylethyl]-N-methyl-(9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ | \\ | \\ | \\ \text{H}_2\text{N}-\text{(CH}_2)}_4-\text{N} \\ | \\ | \\ \text{Me}-\text{CH}-\text{CH}_2 \\ | \\ \text{O} \\ \end{array}$$

RN 547713-16-6 CAPLUS

CN Ethanethioic acid, S-[3-[[2-(1,3-benzodioxol-5-yl)-1-methylethyl]methylamino]propyl] ester (9CI) (CA INDEX NAME)

IT 4764-17-4D, Methylenedioxyamphetamine, N-alkylated

RL: ANT (Analyte); ANST (Analytical study)

(immunoassay, haptens, reagents and kit for determining 3,4-methylenedioxymethamphetamine in body fluids)

RN 4764-17-4 CAPLUS

CN 1,3-Benzodioxole-5-ethanamine, \alpha-methyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \operatorname{NH_2} \\ \operatorname{Me-CH-CH_2} \\ \end{array}$$

#### IT 42542-10-9P, 3,4-Methylenedioxymethamphetamine

RL: ANT (Analyte); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation)

(immunoassay, haptens, reagents and kit for determining 3,4methylenedioxymethamphetamine in body fluids)

42542-10-9 CAPLUS RN

1,3-Benzodioxole-5-ethanamine, N,α-dimethyl- (9CI) (CA INDEX NAME) CN

#### IT 547713-12-2P 547713-14-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(in preparation of hapten; immunoassay, haptens, reagents and kit for determining 3,4-methylenedioxymethamphetamine in body fluids)

547713-12-2 CAPLUS RN

Butanoic acid, 4-[[2-(1,3-benzodioxol-5-yl)-1-methylethyl]methylamino]-, CN ethyl ester (9CI) (CA INDEX NAME)

547713-14-4 CAPLUS RN

1H-Isoindole-1,3(2H)-dione, 2-[4-[[2-(1,3-benzodioxol-5-yl)-1-CN methylethyl]methylamino]butyl]- (9CI) (CA INDEX NAME)

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 4 OF 8 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:155666 CAPLUS

DOCUMENT NUMBER: 136:162629

Ecstasy-class analogs and use of same in TITLE:

detection of ecstasy-class compounds

Rouhani, Riaz; Sanchez, Anthony De Jesus; Davoudzadeh, INVENTOR(S):

David; Coty, William A.; Vistica, Cynthia A.

Microgenics Corporation, USA PATENT ASSIGNEE(S):

Brit. UK Pat. Appl., 89 pp. SOURCE:

CODEN: BAXXDU

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO.             | KIND   | DATE       | API | PLICATION NO. |   | DATE     |  |
|------------------------|--------|------------|-----|---------------|---|----------|--|
|                        |        |            |     |               | _ |          |  |
| GB 2361473             | A1     | 20011024   | GB  | 2001-5517     |   | 20010306 |  |
| GB 2361473             | B2     | 20040901   |     |               |   |          |  |
| DE 10111224            | A1     | 20020221   | DE  | 2001-10111224 |   | 20010308 |  |
| US 2003207469          | A1     | 20031106   | US  | 2003-457314   |   | 20030609 |  |
| PRIORITY APPLN. INFO.: |        |            | US  | 2000-521070   | Α | 20000308 |  |
| OTHER SOURCE (S) .     | маррат | 136.162629 |     |               |   |          |  |

OTHER SOURCE(S): MARPAT 136:162629

The present invention provides a system for the improved detection of ecstasy-class compds. in biol. samples. New ecstasy -class analogs are provided for detection of such ecstasy-class drugs. These analogs are compds. or salts thereof, of a 2-amino-methylenedioxyphenyl derivative attached to Z, where Z is a moiety capable of bonding, either directly or indirectly, with an immunogenic carrier, a detectable label, or a solid capture vehicle. Such analogs may be used to construct immunogens , enzyme or enzyme-donor conjugates, and other conjugates. The immunogens reproducible generate antibodies with an exquisite ability to distinguish various ecstasy-class drugs in biol. samples from potentially interfering substances. The specific antibodies and conjugates may be used to distinguish and measure various ecstasy-class compds. in biol. samples, such as those obtained from an individual suspected of substance abuse. In another aspect, the invention includes certain reagents, reagent combinations, and kits for performing assay methods for ecstasy-class compds. in a biol. sample.

IT 42542-10-9, Ecstasy 42542-10-9D,

Ecstasy, analogs 82801-81-8, N-Ethyl-3,4-

methylenedioxyamphetamine

RL: ANT (Analyte); ANST (Analytical study)

(ecstasy-class analogs and use of same in detection

of ecstasy-class compds.)

RN 42542-10-9 CAPLUS

CN 1,3-Benzodioxole-5-ethanamine,  $N,\alpha$ -dimethyl- (9CI) (CA INDEX NAME)

RN 42542-10-9 CAPLUS

CN 1,3-Benzodioxole-5-ethanamine,  $N,\alpha$ -dimethyl- (9CI) (CA INDEX NAME)

CN 1,3-Benzodioxole-5-ethanamine, N-ethyl- $\alpha$ -methyl- (9CI) (CA INDEX NAME)

IT 397334-21-3P

RL: BSU (Biological study, unclassified); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)

(ecstasy-class analogs and use of same in detection
of ecstasy-class compds.)

RN 397334-21-3 CAPLUS

CN 1H-Pyrrole-2,5-dione, 1-[4-[[2-(1,3-benzodioxol-5-yl)-1-methylethyl]amino]butyl]- (9CI) (CA INDEX NAME)

IT 397334-20-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(ecstasy-class analogs and use of same in detection
of ecstasy-class compds.)

RN 397334-20-2 CAPLUS

CN 1,4-Butanediamine, N-[2-(1,3-benzodioxol-5-yl)-1-methylethyl]- (9CI) (CA INDEX NAME)

IT 397334-19-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (ecstasy-class analogs and use of same in detection
 of ecstasy-class compds.)

RN 397334-19-9 CAPLUS

CN Carbamic acid, [4-[[2-(1,3-benzodioxol-5-yl)-1-methylethyl]amino]butyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

L19 ANSWER 5 OF 8 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1994:127568 CAPLUS

DOCUMENT NUMBER: 120:127568

TITLE: Dual analyte immunoassay for amphetamine and

methamphetamine

INVENTOR(S): Ordonez, Kathy Palmer; Salamone, Salvatore Joseph

PATENT ASSIGNEE(S): F. Hoffmann-La Roche A.-G., Switz.

SOURCE: Eur. Pat. Appl., 12 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO.             | KIND       | DATE         | APPLICATION NO.       | DATE       |
|------------------------|------------|--------------|-----------------------|------------|
| EP 574782              | A2         | 19931222     | EP 1993-109091        | 19930607   |
| EP 574782              | <b>A</b> 3 | 19940209     |                       |            |
| EP 574782              | В1         | 19981021     |                       |            |
| R: BE, CH, DE,         | DK, ES     | , FR, GB, GF | R, IE, IT, LI, LU, NL | , PT       |
| CA 2096495             | AA         | 19931217     | CA 1993-2096495       | 19930518   |
| CA 2096495             | С          | 20020709     |                       |            |
| ES 2123589             | Т3         | 19990116     | ES 1993-109091        | 19930607   |
| JP 06094711            | A2         | 19940408     | JP 1993-143841        | 19930615   |
| JP 2726793             | B2         | 19980311     |                       |            |
| US 5501987             | Α          | 19960326     | US 1994-258125        | 19940610   |
| PRIORITY APPLN. INFO.: |            |              | US 1992-899196        | A 19920616 |
| OTHER SOURCE(S):       | MARPAT     | 120:127568   |                       |            |

amphetamine and methamphetamine is provided in which
only one labeled binding partner is used which can interact with the
combination of antibodies and their corresponding analytes
detecting the presence of the analytes either alone or in
combination. The binding partner is a labeled derivative of one of the
analytes capable of binding to both antibodies with different

affinity. Preparation of of an amphatamine derivative label, a BSA conjugate, and microparticles sensitized with the conjugate are described. A standard curve for the assay is included, as are cross-reactivity data for amphetamine-related drugs.

### IT 4764-17-4, Methylenedioxyamphetamine 42542-10-9

A dual analyte immunoassay for the detection of

## , Methylenedioxymethamphetamine

RL: ANST (Analytical study)

(cross-reactivity of, in amphetamine/methamphetamine immunoassay with single labeled analyte derivative)

RN 4764-17-4 CAPLUS

CN 1,3-Benzodioxole-5-ethanamine, α-methyl- (9CI) (CA INDEX NAME)

RN 42542-10-9 CAPLUS

CN 1,3-Benzodioxole-5-ethanamine, N,α-dimethyl- (9CI) (CA INDEX NAME)

L19 ANSWER 6 OF 8 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1992:147517 CAPLUS

DOCUMENT NUMBER:

116:147517

TITLE:

Phencyclidine and phencyclidine metabolite assays,

tracers, immunogens, antibodies

and reagent kit

INVENTOR(S):

Dubler, Robert Edward; Frintner, Mary Pat; Grote, Jonathan; Hawksworth, David James; Nam, Daniel S.; Wray, Larry Kay; Hadley, Gregg Allen; Hopkins, Hal

Dayton; Ungemach, Frank S.

PATENT ASSIGNEE(S):

SOURCE:

Abbott Laboratories, USA

Eur. Pat. Appl., 34 pp. CODEN: EPXXDW

DOCUMENT TYPE:

LANGUAGE:

Patent English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

| PATENT NO.             | KIND   | DATE      | APPLICATION NO. | DATE        |
|------------------------|--------|-----------|-----------------|-------------|
| EP 459387              | A2     | 19911204  | EP 1991-108674  | 19910528    |
|                        |        |           | EP 1991-1000/4  | 19910320    |
| EP 459387              | A3     | 19920902  |                 |             |
| EP 459387              | B1     | 19950920  |                 |             |
| R: AT, BE, CH,         | DE, ES | , FR, GB, | IT, LI, NL      |             |
| US 5155212             | Α      | 19921013  | US 1990-529988  | 19900529    |
| AU 9177272             | A1     | 19911205  | AU 1991-77272   | 19910522    |
| AU 643524              | B2     | 19931118  |                 |             |
| CA 2043372             | AA     | 19911130  | CA 1991-2043372 | 19910528    |
| AT 128241              | E      | 19951015  | AT 1991-108674  | 19910528    |
| ES 2080188             | Т3     | 19960201  | ES 1991-108674  | 19910528    |
| JP 04235199            | A2     | 19920824  | JP 1991-125955  | 19910529    |
| us 5407834             | Α      | 19950418  | US 1992-831762  | 19920427    |
| PRIORITY APPLN. INFO.: |        |           | US 1990-529988  | A 19900529  |
|                        |        |           | US 1986-866193  | B2 19860521 |

OTHER SOURCE(S): MARPAT 116:147517

AB The present invention is directed to a fluorescence polarization assay for phenylcyclidine and phenylcyclidine derivs., to the various components needed for preparing and carrying out such an assay, and to methods of making these components. Specifically, tracers, immunogens and (monoclonal) antibodies are disclosed, as well as methods for making them, and a reagent kit containing them. The tracers and the

immunogens are made from substituted phencyclidine compds. A
fluorescein moiety is included in the tracer, while a poly(amino acid)
forms a part of the immunogen. The assay is conducted by
measuring the degree of polarization retention of plane polarized light
that has been passed through a sample containing antiserum and tracer. The
assay has a high degree of specificity for phencyclidine and metabolites
and analogs thereof, while minimizing mass reactivity to a host of other
synthetic metabolites and naturally occurring compds.

IT 4764-17-4 42542-10-9 82801-81-8

RL: ANST (Analytical study)

(phencyclidine fluorescence polarization immunoassay crossreactivity to)

RN 4764-17-4 CAPLUS

CN 1,3-Benzodioxole-5-ethanamine,  $\alpha$ -methyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c} ^{\rm NH_2} \\ | \\ ^{\rm Me-CH-CH_2} \end{array}$$

RN 42542-10-9 CAPLUS

CN 1,3-Benzodioxole-5-ethanamine, N, $\alpha$ -dimethyl- (9CI) (CA INDEX NAME)

RN 82801-81-8 CAPLUS

CN 1,3-Benzodioxole-5-ethanamine, N-ethyl- $\alpha$ -methyl- (9CI) (CA INDEX NAME)

L19 ANSWER 7 OF 8 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

1991:577279 CAPLUS

DOCUMENT NUMBER:

115:177279

TITLE:

Reagents, methods, and kits for an amphetamine

-class fluorescence polarization immunoassay

INVENTOR(S):

Brynes, Paul Jeffrey; Johnson, Donald Duane; Molina,

Cynthia Martha; Flentge, Charles Arthur; Jonas,

Patrick F.

PATENT ASSIGNEE(S):

Abbott Laboratories, USA

SOURCE:

Eur. Pat. Appl., 30 pp.

CODEN: EPXXDW

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

### PATENT INFORMATION:

|      | PATENT NO.         | KIND | DATE     | APPLICATION NO. | DATE        |
|------|--------------------|------|----------|-----------------|-------------|
|      | EP 399184          | A2   | 19901128 | EP 1990-106319  | 19900403    |
|      | EP 399184          | A3   | 19911227 |                 |             |
|      | EP 399184          | В1   | 19950913 |                 |             |
|      | R: DE, ES, FR,     | IT   |          |                 |             |
|      | US 5101015         | Α    | 19920331 | US 1989-335627  | 19890410    |
|      | ES 2079390         | Т3   | 19960116 | ES 1990-106319  | 19900403    |
|      | JP 02300663        | A2   | 19901212 | JP 1990-93823   | 19900409    |
|      | JP 2894782         | B2   | 19990524 |                 |             |
|      | CA 2014318         | AA   | 19901010 | CA 1990-2014318 | 19900410    |
|      | CA 2014318         | С    | 20000808 |                 |             |
|      | US 5248791         | Α    | 19930928 | US 1992-820729  | 19920114    |
|      | US 5354693         | Α    | 19941011 | US 1993-83928   | 19930629    |
| PRIO | RITY APPLN. INFO.: |      |          | US 1989-335627  | A 19890410  |
|      |                    |      |          | US 1992-820729  | A3 19920114 |
|      |                    |      |          |                 |             |

OTHER SOURCE(S): MARPAT 115:177279

A fluorescence polarization immunoassay (FPIA) for detecting the presence of ≥1 amphetamine-class analytes in a test sample is provided. The immunoassay uses competition between the analyte and a fluorescently labeled tracer for the binding site on an antibody specific for phenethylamine derivs. The concentration of amphetamine-class analyte in the sample dets. the amount of tracer that binds to the antibody. The amount of tracer/antibody complex formed can be quant. measured and is inversely proportional to the quantity of analyte in the test sample. Also provided are tracers, immunogens used to elicit antibodies for use as assay reagents, and assay kits incorporating these tracers and assay reagents. Thus, N-tert-butoxycarbonyl-N-carboethoxymethyl-d,lamphetamine was prepared and used to prepare a N-carboxymethyl-d,lamphetamine-albumin conjugate for use as immunogen. Synthesis of N-acetamidomethylfluorescein-d,l-amphetamine for use as a tracer is described, as is preparation of other tracers and immunogenic conjugates. The FPIA and reagents of the invention had sufficient cross-reactivity to detect amphetamine -class drugs at concns. which produce a stimulating or toxic effect. At the same time, concns. of phenethylamine-like substances common in certain foods (e.g. tryptamine and tyramine) were not readily detected. Pretreatment of test samples with riboflavin-binding protein decreased the background intensity of the samples.

IT 4764-17-4, 3,4-Methylenedioxyamphetamine
42542-10-9, 3,4-Methylenedioxymethamphetamine
82801-81-8, N-Ethyl-3,4-Methylenedioxyamphetamine
RL: ANT (Analyte); ANST (Analytical study)
(detection of, by fluorescence-polarization immunoassay)
RN 4764-17-4 CAPLUS

CN 1,3-Benzodioxole-5-ethanamine,  $\alpha$ -methyl- (9CI) (CA INDEX NAME)

RN 42542-10-9 CAPLUS CN 1,3-Benzodioxole-5-ethanamine, N,α-dimethyl- (9CI) (CA INDEX NAME)

RN 82801-81-8 CAPLUS

CN 1,3-Benzodioxole-5-ethanamine, N-ethyl- $\alpha$ -methyl- (9CI) (CA INDEX NAME)

L19 ANSWER 8 OF 8 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

1991:464728 CAPLUS

DOCUMENT NUMBER:

115:64728

TITLE:

Method, tracers, and reagents for immunochemical

detection of amphetamine and/or d-

methamphetamine or other phenethylamines in

biological samples

INVENTOR(S):

Heiman, Daniel Feulner; Hsiang-Yun, Yang Hu; Johnson,

Sharon Ann

PATENT ASSIGNEE(S):

Abbott Laboratories, USA

SOURCE:

Eur. Pat. Appl., 49 pp.

CODEN: EPXXDW

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

| PATENT NO. |      |      |                 | KIND |     | DATE       |                 | Ī    | APPLICATION NO. |     |            |              | DATE         |   |          |  |
|------------|------|------|-----------------|------|-----|------------|-----------------|------|-----------------|-----|------------|--------------|--------------|---|----------|--|
|            | EP   | 3712 | - <b></b><br>53 |      |     | A2         |                 | 1990 | 0606            | ]   | EP         | 1989-119701  |              | • | 19891024 |  |
|            | EΡ   | 3712 | 53              |      |     | <b>A3</b>  |                 | 1990 | 0620            |     |            |              |              |   |          |  |
|            | EΡ   | 3712 | 53              |      |     | B1         |                 | 1995 | 0913            |     |            |              |              |   |          |  |
|            |      | R:   | AT,             | BE,  | CH, | DE,        | ES,             | FR,  | GB,             | IT, | $_{ m LI}$ | , NL         |              |   |          |  |
|            | ES   | 2079 | 368             |      |     | Т3         |                 | 1996 | 0116            | ]   | ES         | 1989-119701  |              |   | 19891024 |  |
|            | AU   | 8943 | 807             |      |     | <b>A</b> 1 |                 | 1990 | 0503            | Ž   | ΑU         | 1989-43807   |              |   | 19891026 |  |
|            | ΑU   | 6349 | 85              |      |     | B2         |                 | 1993 | 0311            |     |            |              |              |   |          |  |
|            | CA   | 2001 | 696             |      |     | AA         |                 | 1990 | 0428            | (   | CA         | 1989-2001696 | <del>,</del> |   | 19891027 |  |
|            | JΡ   | 0217 | 0050            |      |     | A2         |                 | 1990 | 0629            | ,   | JP         | 1989-281627  |              |   | 19891028 |  |
|            | US   | 5262 | 333             |      |     | Α          |                 | 1993 | 1116            | 1   | US         | 1992-898238  |              |   | 19920612 |  |
| PRIOF      | RITY | APP  | LN.             | INFO | .:  |            |                 |      |                 | 1   | US         | 1988-265361  |              | Α | 19881028 |  |
| OTHER      | R SC | URCE | (S):            |      |     | MARE       | TA <sup>9</sup> | 115: | 64728           | 3   |            |              |              |   |          |  |
| GT         |      |      |                 |      |     |            |                 |      |                 |     |            |              |              |   |          |  |

- \* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT \*
- AB The title method, reagents, and tracers are used for determining amphetamine (I) and d-methamphetamine (II) in a biol. fluid, e.g. urine. The method can also detect certain "designer drugs", e.g. 3,4-methylenedioxyamphetamine. An improved

fluorescence polarization immunoassay is provided for determining I and II in a single assay. The procedure includes pretreatment of the biol. sample with (1) aqueous IO4- solution to eliminate cross-reactants, e.g. hydroxyphenethylamine, and (2) riboflavin-binding protein to reduce fluorescence interference from riboflavin. Also provided are tracer compds., e.g. III (Q = fluorescein or fluorescein derivative; Z = NH, CO, SO2; R = linking group including ≤5 heteroatoms and a total of 0-15 C atoms and heteroatoms); preparation of the tracer compds. is described. An automatic assay apparatus and kit for performing the method of the invention are also described, as is the preparation of immunogens for production of antibodies for the immunoassay. Thus, tracers IV and V were prepared and used in an immunoassay for determination of I and II. Cross-reactivity of the immunoassay for tyramine was .apprx.0.4% and for l-methamphetamine was <5%.

4764-17-4, 3,4-Methylenedioxyamphetamine 42542-10-9, 3,4-Methylenedioxymethamphetamine 82801-81-8

RL: ANT (Analyte); ANST (Analytical study)
(determination of, by fluorescence polarization immunoassay)

RN 4764-17-4 CAPLUS

CN 1,3-Benzodioxole-5-ethanamine, \alpha-methyl- (9CI) (CA INDEX NAME)

RN 42542-10-9 CAPLUS CN 1,3-Benzodioxole-5-ethanamine, N, $\alpha$ -dimethyl- (9CI) (CA INDEX NAME)

RN 82801-81-8 CAPLUS CN 1,3-Benzodioxole-5-ethanamine, N-ethyl- $\alpha$ -methyl- (9CI) (CA INDEX NAME)

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FULL ESTIMATED COST ENTRY SESSION 66.52 728.82

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chain nodes :
10 11 12 13 22
ring nodes :
1 2 3 4 5 6 7 8 9
chain bonds :
1-22 5-10 10-11 11-12 11-13
ring bonds :
1-2 1-6 2-3 2-9 3-4 3-7 4-5 5-6 7-8 8-9
exact/norm bonds :
1-22 11-12
exact bonds :
2-9 3-7 5-10 7-8 8-9 10-11 11-13
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :

containing 1:

G1:H,CH3,Et

G2:CH3,Et,H

G3:0,S,N

Hydrogen count :

1:= exact 1 4:= exact 1 6:= exact 1 8:= exact 2 10:= exact 2 11:= exact 1

13:= exact 3
Match level:

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS

11:CLASS 12:CLASS 13:CLASS 22:CLASS

L20 STRUCTURE UPLOADED

=> s 120

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100.0% PROCESSED 9 ITERATIONS 0 ANSWERS

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FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 9 TO 360

PROJECTED ANSWERS: 0 TO 0

L21 0 SEA SSS SAM L20

=> s 121 sss full

FULL SEARCH INITIATED 12:55:00 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 144 TO ITERATE

100.0% PROCESSED 144 ITERATIONS 0 ANSWERS

SEARCH TIME: 00.00.01

L22 0 SEA SSS FUL L20

=> FIL CAPLUS

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FULL ESTIMATED COST 161.33 890.15

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FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

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